

Doppler shift on local density of states and local impurity scattering in the vortex state

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Abstract

The vortex state thermal and transport properties of the high T_c copper oxides can be understood in a d -wave gap model and are dominated by the extended quasiparticle states that exist along the nodal directions in momentum space. The Doppler shift on these states due to the circulating supercurrents around the vortex core, introduces new van Hove ridges into the energy dependent local density of states (LDOS) as a function of distance in the region between cores. We emphasize the topology of these ridges and the effect on them of local static impurity scattering in Born and unitary limit. We treat possible orthorhombicity. Effective local scattering rates are also obtained.

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I. INTRODUCTION

The theoretical predictions of Volovik^{1,2} and Kopnin and Volovik^{3,4} that the low temperature specific heat in a d -wave superconductor would vary as the square root of the applied magnetic field (\sqrt{H}) was verified in several experiments.^{5–9} To understand the experimental data it is assumed that the extended quasiparticle states outside the vortex cores can be treated semiclassically taking account only of the Doppler shift due to the circulating supercurrents. To obtain the specific heat, which is a bulk property of the system, it is necessary to carry out a spacial average over the vortex unit cell of the local density of states (LDOS) which varies as a function of distance from the vortex core center. The low temperature limit of the specific heat depends on the zero frequency limit of this averaged density of quasiparticle states. This quantity is not only affected by the magnetic field \mathbf{H} but can also depend on impurity content,^{10,11} particularly in the resonant scattering limit. In this limit the theory of a d -wave superconductor without magnetic field predicts a finite, constant value for its zero frequency limit which is proportional to the self consistent effective scattering rate and this leads to the well known universal limit for the transport.^{12–15}

When the magnetic field is oriented in the copper oxide plane rather than perpendicular to it new anisotropy effects in the specific heat are predicted.^{11,16–18} In addition transport properties are also affected by the Doppler shift of a vortex state.^{18,19} The thermal conductivity has been particularly widely studied.^{19–25}

The semiclassical Doppler shift of the electron due to the circulating supercurrents outside the vortex core should also affect the frequency dependence of the LDOS which can be measured in scanning tunneling microscope (STM) experiments. In view of the above successes in our understanding of the thermal and transport properties of the copper oxides it is of interest to understand the signature of the Doppler shift on the LDOS and the effect of impurities on it. Very recently Franz and Tešanović²⁶ considered the LDOS problem and compared an average over vortex winding angles of the semi classical LDOS with equivalent results obtained from complete solutions of the BdG equations for a single vortex. Their main conclusion was that the semiclassical approach does indeed provide a

good approximation for this quantity.

For no magnetic field ($H = 0$) there is a single van Hove singularity in the density of states at energy ω equal to the gap amplitude which does not shift with position \mathbf{r} (homogeneous case). For finite H new van Hove ridges are predicted. The actual number of such ridges and their topology depends on the winding angel β and simple formulas can be obtained from which their contour in (ω, \mathbf{r}) -space can be traced. The effect of impurities on the topology of these ridges is considered as is the effect of orthorhombicity. Impurities are treated in both Born and unitary limit, and the influence of the circulating supercurrents on the local effective impurity scattering is also considered. This topic was recently discussed by Barash and Svidzinskii.²⁷ Orthorhombicity, present in $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$ (YBCO) because of the existence of chains, is treated within a simple effective mass model for the in-plane electronic dispersion curves and a possible subdominant s -wave component is added to the dominant d -wave gap.

The tetragonal case is the subject of section II. Impurities are included. Generalization to the orthorhombic case is given in section III. Section IV deals with effective local impurity scattering rates. A short conclusion is found in section V.

II. TETRAGONAL CASE

In a semiclassical approximation the local Green's function at position \mathbf{r} is given in terms of the Doppler shift $\mathbf{v}_F(\mathbf{k})\mathbf{q}_s$ by

$$G(\mathbf{k}, \omega_n; \mathbf{r}) = -\frac{[i\omega_n - \mathbf{v}_F(\mathbf{k})\mathbf{q}_s] \tau_0 + \varepsilon_{\mathbf{k}}\tau_3 + \Delta_{\mathbf{k}}\tau_1}{[\omega_n + i\mathbf{v}_F(\mathbf{k})\mathbf{q}_s]^2 + \varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} \quad (1)$$

where $\tau_{1,2,3}$ are the 2×2 Pauli matrices, $i\omega_n$ the Matsubara frequencies $i(2n+1)\pi T$, $n = 0, \pm 1, \pm 2, \dots$ and T is the temperature. The electronic dispersion in momentum space \mathbf{k} is $\varepsilon_{\mathbf{k}}$ and the gap in the two-dimensional copper oxide Brillouin zone is $\Delta_{\mathbf{k}}$. The electronic Fermi velocity is $\mathbf{v}_F(\mathbf{k})$ and \mathbf{q}_s is the momentum associated with the superfluid flow about the vortex. In the magnetic field region $H_{c1} < |\mathbf{H}| \ll H_{c2}$ with $H_{c1,2}$ the lower and upper critical field respectively, and \mathbf{H} the external magnetic field taken to be perpendicular to the

CuO₂-planes, the intervortex distance $R = \frac{1}{a}\sqrt{\frac{\phi_0}{\pi|\mathbf{H}|}}$ where a is a geometrical factor of order one which is associated with the vortex arrangement, and ϕ_0 is the fundamental quantum of flux. In what follows, the position \mathbf{r} will be measured relative to the center of the vortex core. We use polar coordinates (r, β) with β the vortex winding angle. The dimensionless variable $\rho = r/R$ takes on the value 1 at the boundary of the vortex unit cell. It is expected that $R \gg \xi_0$ (ξ_0 is the coherence length) and we will be interested only in values of $r > \xi_0$.

Assuming a circular velocity field for the supercurrents around a single vortex, $\mathbf{v}_s = \frac{\hbar\hat{\beta}}{2mr}$ with $\hat{\beta}$ a unit vector along the current, the Doppler shift

$$\mathbf{v}_F(\mathbf{k})\mathbf{q}_s = \frac{E_H}{\rho} \sin(\phi - \beta), \quad (2)$$

where E_H is the magnetic energy scale that enters our problem and is equal to $\frac{a}{2}v_F\sqrt{\frac{\pi H}{\phi_0}} \equiv \nu\Delta_0$ where the last identity measures E_H in units of the gap amplitude Δ_0 . In Eq. (2) ϕ is the polar angle associated with momentum \mathbf{k} on the Fermi surface and the d -wave gap $\Delta_{\mathbf{k}} = \Delta_0 \cos 2\phi \equiv \Delta_d(\phi)$ in the same model.

The local quasiparticle density of states at relative position ρ and energy ω , $N_L(\rho, \omega)$, follows directly from the analytic continuation of G defined in Eq. (1) to real frequencies $i\omega_n \rightarrow \omega + i0^+$ with

$$\frac{N_L(\rho, \omega)}{N_0} = \int_0^{2\pi} \frac{d\phi}{2\pi} \Re \left\{ \frac{|\omega - \mathbf{v}_F(\mathbf{k})\mathbf{q}_s|}{\sqrt{[\omega - \mathbf{v}_F(\mathbf{k})\mathbf{q}_s]^2 - \Delta_d^2(\phi)}} \right\}, \quad (3)$$

where N_0 is the normal state density of states. Note that the Doppler shift of Eq. (2) which enters (3) depends on the magnetic field $|\mathbf{H}| = H$ through $E_H \sim \sqrt{H}$ and on the position of the STM tip away from the vortex core given by ρ and β . We will be interested only in the region where \mathbf{r} is outside the vortex core of size ξ_0 . This is mandated by the fact that our approach does not treat in detail the core interior but instead includes only the supercurrents outside the core through the superfluid velocity field $\mathbf{v}_s = \frac{\hbar\hat{\beta}}{2mr}$ which itself is an approximation. Nevertheless, it is the aim of this work to understand how the presence of \mathbf{v}_s modifies the LDOS in the region between the vortex cores.

The integral in Eq. (3) is easily evaluated. We present a first set of results which include some impurity scattering in Born approximation. This smooths out the logarithmic

singularity at the gap amplitude predicted for pure d -wave with $H = 0$. To include static impurity scattering it is simply necessary to exchange the frequency ω and the gap $\Delta_d(\phi)$ in Eq. (3) by their renormalized values denoted by a tilde, i.e.: $\tilde{\omega}$ and $\tilde{\Delta}(\phi)$. The renormalized frequency

$$\tilde{\omega}(\rho, \beta, \omega) = \omega + i\pi t^+ \Omega(\rho, \beta, \omega) \quad (4)$$

in Born approximation with t^+ the impurity scattering rate in the normal state, and

$$\tilde{\omega}(\rho, \beta, \omega) = \omega + i\pi \Gamma^+ \frac{\Omega(\rho, \beta, \omega)}{\Omega^2(\rho, \beta, \omega) + D^2(\rho, \beta, \omega)} \quad (5)$$

in the unitary limit with Γ^+ replacing t^+ of Eq. (4). The renormalized gap $\tilde{\Delta}(\phi) = \Delta_0 \cos 2\phi + i\tilde{\Delta}_s(\rho, \beta, \omega)$ in a $(d + is)$ -wave symmetry with

$$\tilde{\Delta}_s(\rho, \beta, \omega) = i\pi t^+ D(\rho, \beta, \omega) \quad (6)$$

for Born scattering and

$$\tilde{\Delta}_s(\rho, \beta, \omega) = i\pi \Gamma^+ \frac{D(\rho, \beta, \omega)}{\Omega^2(\rho, \beta, \omega) + D^2(\rho, \beta, \omega)} \quad (7)$$

in the unitary limit. Here, the two functions $\Omega(\rho, \beta, \omega)$ and $D(\rho, \beta, \omega)$ are

$$\Omega(\rho, \beta, \omega) = \left\langle \frac{\tilde{\omega}(\rho, \beta, \omega) - \mathbf{v}_F(\mathbf{p})\mathbf{q}_s}{\sqrt{[\tilde{\omega}(\rho, \beta, \omega) - \mathbf{v}_F(\mathbf{p})\mathbf{q}_s]^2 - \tilde{\Delta}_s^2(\rho, \beta, \omega) - \Delta_d^2(\phi)}} \right\rangle_\phi \quad (8)$$

and

$$D(\rho, \beta, \omega) = \left\langle \frac{\tilde{\Delta}_s(\rho, \beta, \omega)}{\sqrt{[\tilde{\omega}(\rho, \beta, \omega) - \mathbf{v}_F(\mathbf{p})\mathbf{q}_s]^2 - \tilde{\Delta}_s^2(\rho, \beta, \omega) - \Delta_d^2(\phi)}} \right\rangle_\phi, \quad (9)$$

where $\langle \dots \rangle_\phi$ indicates an angular average over the angles ϕ around the circular Fermi surface in the two-dimensional copper oxide Brillouin zone.

In the top frame of Fig. 1 we show our results for a d -wave superconductor (tetragonal symmetry) with a gap amplitude $\Delta_0 = 24$ meV. We take the magnetic field $\mathbf{H} \parallel c$ -axis, i.e. \mathbf{H} is perpendicular to the copper oxygen planes and the vortex winding angle $\beta = 0^\circ$. The vertical axis is labeled by $N_L(\rho, \omega)$ which is given by

$$N_L(\rho, \omega) = \Re \{ \Omega(\rho, \beta, \omega) \}_{\beta=\text{const}}, \quad (10)$$

and features the LDOS as a function of ρ and ω . Estimates of the magnetic energy scale E_H in YBCO have been considered by Vekhter et al.¹⁷ This quantity is not very well known but best estimates give between

$$E_H = 20 - 30[\text{K}] \sqrt{H[\text{Tesla}]}.$$

Therefore the magnetic energy scale has been set at 10% of the gap amplitude for illustrative purposes, i.e. $\nu = 0.1$ in our notation and the static impurity content in Born approximation is $t^+ = 0.1 \text{ meV}$, enough to smear out the van Hove singularity but not enough to make them disappear. (This value of t^+ corresponds to a scattering rate of about 6 K. Recent experiments by Hosseini et al.²⁸ seem to indicate an even smaller scattering rate.) Three prominent sets of ridges are seen for ρ in the range 0.1 (at the vortex core, i.e. at $r = \xi_0$) and 1.0 (at the vortex cell boundary). The case with no magnetic field is shown as the bottom frame of Fig. 1 for comparison. Only one prominent van Hove ridge is seen in this second case and it is centered at $\omega = \Delta_0 = 24 \text{ meV}$ and, of course, there is no ρ dependence since there is no vortex core and thus no spatial inhomogeneities in the problem. A main ridge around $\omega = 24 \text{ meV}$ is still seen in the top frame although as ρ is decreased and the vortex core is approached at $\rho = 0.1$ it has shifted in energy significantly. The other two ridges are due entirely to the Doppler shift provided by the supercurrents and can be understood as follows. In the pure case (no impurity scattering) the ridges in $N_L(\rho, \omega)$ correspond to extrema in the zeros of the denominator of Eq. (3), i.e. they correspond to the extrema of the equation

$$\omega = \mathbf{v}_F(\mathbf{k})\mathbf{q}_s \pm \Delta(\phi) = \Delta_0 \left[\frac{\nu}{\rho} \sin(\phi - \beta) \pm \cos 2\phi \right], \quad (11)$$

i.e. to solutions of equation

$$\frac{d\omega}{d\phi} = 0 = \frac{\nu}{\rho} \cos(\phi - \beta) \mp 2 \sin 2\phi, \quad (12)$$

which have been written for a general value of vortex winding angle β . There are three solutions of this equation for the case considered in the top frame of Fig. 1 ($\beta = 0$). The

critical values of frequency ω_{ci} with $i = 1, 2, 3$ are shown as a function of distance from the vortex core ρ in the top frame of Fig. 2. For $\omega \geq 0$ the solutions occur at the critical angles $\phi_{c1,2} = \pm\pi/2$ and $\phi_{c3} = \sin^{-1}(\nu/4\rho)$ respectively and the corresponding values of ω_{ci} are

$$\omega_{c1,2} = \Delta_0(1 \pm \nu/\rho), \quad (13)$$

which are valid without restriction; in the limit $\nu/\rho \rightarrow 0$ we find

$$\omega_{c3} = \Delta_0 \left[1 + \frac{1}{2} \left(\frac{\nu}{2\rho} \right)^2 \right]. \quad (14)$$

Numerical solutions can always be obtained and are needed except for a few simple cases. For $\nu = 0$, no magnetic field, all $\omega_{ci} = \Delta_0$ as expected. At the vortex cell boundary $\rho = 1$, i.e. $r = R$, the three critical frequencies are in units of Δ_0 1.1, 0.9, and 1.0013 respectively, and at the vortex core which corresponds to $\rho = 0.1$ for $\nu = 0.1$ these values are 2, 0, and 1.125. These expectations are bourn out in the top frame of Fig. 1. We note from Eq. (13) that the spacing of the two additional structures away from $\omega = \Delta_0$ goes in the antinodal direction ($\beta = 0^\circ$) like

$$\omega_{c1,2} \propto \sqrt{H},$$

i.e. is linear in ν ; the shift of the main van Hove ridge from Δ_0 due to the Doppler shift goes instead like

$$\omega_{c3} \propto H,$$

i.e. is linear in the magnetic field in the limit $\nu/\rho \rightarrow 0$. Other directions, $\beta \neq 0^\circ$, will develop other H -dependencies of the spacing of the van Hove ridges which will have to be evaluated numerically in most cases.

Also note the $\omega \rightarrow 0$ limit of the LDOS. It goes to zero linearly in the $H = 0$ case but, in contrast, it takes on a finite value when vortices are present. Its value depends strongly on position ρ in the vortex unit cell and increases strongly with decreasing ρ . It is the average of the LDOS at $\omega = 0$ over the vortex unit cell, i.e. the average over ρ and winding angle β that determines the low temperature bulk specific heat and this varies with the value of H .

Franz and Tešanović²⁶ discuss in detail how this region of small ω can be strongly modified by an in-plane angular dependence to the tunneling matrix element that comes into the relationship between STM measurements and the LDOS itself. These are only the same when the tunneling element is constant.

In the bottom frame of Fig. 2 we show again the same data as shown in the top frame of Fig. 1 but in a different representation which allows to see the ridges a little more clearly. What is presented here is $N_L(\rho, \omega)$ vs. ω for fixed values of ρ , namely $\rho = 0.2$ (solid line), $\rho = 0.3$ (dashed line), $\rho = 0.6$ (dotted line), and $\rho = 1.0$ (dash-dotted line). The vortex core radius equal to the coherence length ξ_0 corresponds to $\rho = 0.1$ and the inter vortex distance is $\rho = 1.0$. Finally, a thin solid line indicates $N_L(\omega)$ for no magnetic field, $H = \nu = 0$.

Furthermore, the data shows clearly the main van Hove singularity around, but not precisely at $\omega \simeq \Delta_0$, with some variation with ρ as detailed in the top frame of Fig. 2 (solid line, ω_{c3}). This peak exists even when $H = 0$ (light solid line) when there are no supercurrents and it is the usual d -wave gap peak. Note that here we have included some small amount of impurity scattering in Born approximation, namely $t^+ = 0.1$ meV. The other secondary peaks above and below $\omega \simeq 24$ meV are due to the supercurrents and are the semiclassical signature of the resulting Doppler shifts. (Similar ridges with somewhat different geometry appear in earlier work which makes use of the semiclassical Eilenberger approach.^{29–32} This approach should be better inside the core, a region we do not treat properly. Other related work in the s -wave case is the very recent paper by Eschrig et al.³³) As the STM tip is moved more towards the vortex core, the secondary peak at low energy becomes fairly prominent and also the $\omega = 0$ limit becomes finite as noted before. The topology of the surface $N_L(\rho, \omega)$ vs. ρ and ω is affected by several external variables such as the magnitude of the magnetic field, the vortex winding angle, the type of impurities involved, i.e. Born or unitary scattering, and its strength as we now detail.

The ridge structure in the LDOS changes considerably as the position of the STM tip is changed. This is illustrated in the top frame of Fig. 3 where we show our result for a winding angle $\beta = 45^\circ$, i.e. in the nodal direction. There are striking differences with the

top frame of Fig. 1. Only two ridges are now seen in contrast to three in the $\beta = 0^\circ$ case (the antinodal direction), and the main gap peak around $\omega = 24 \text{ meV}$ at the vortex cell boundary $\rho = 1$ (at $r = R$) moves downward in energy as ρ is reduced toward the vortex core. The $\omega = 0$ value of $N_L(\rho, \omega)$ near $\rho = 0.1$, i.e. $r = \xi_0$, is also much smaller than in the $\beta = 0^\circ$ case.

In the bottom frame of Fig. 3 we show our solutions for the critical values of ω ($\omega_{ci}, i = 1, 2$) which locate the ridges in the top frame. The critical angles $\phi_{ci}, i = 1, 2$ at which the extrema responsible for the ridges occur are also presented as functions of the distance from the vortex center ρ in this frame. It is obvious that geometry strongly affects the topology of the $N_L(\rho, \omega)$ surface.

Impurity scattering can also affect things in an important way. In Fig. 4 we show results for the LDOS $N_L(\rho, \omega)$ as a function of the distance to the vortex core ρ and energy ω for a magnetic energy $\nu = 0.1$, $\mathbf{H} \parallel c$ -axis, and a winding angle $\beta = 0^\circ$ (antinodal direction). This figure is to be compared directly with the top frame of Fig. 1 as the only difference between the two figures is that in Fig. 3 the unitary impurity limit is used, Eqs. (5) and (7), with $\Gamma^+ = 0.1 \text{ meV}$ instead of the Born limit, Eqs. (4) and (6), with $t^+ = 0.1 \text{ meV}$. The structure of the ridges is now more pronounced and the zero frequency limit of the LDOS near the vortex cell boundary is now larger.

III. ORTHORHOMBICITY

YBCO is orthorhombic because of the existence of chains along the b -axis in one of the three copper oxide two-dimensional planes per unit cell. This implies that the gap is in principle a mixture of s - and d -wave symmetry which do belong to the same irreducible representation of the crystal lattice group, and therefore has the form

$$\Delta(\phi) = \Delta_0 (\cos 2\phi + s) \quad (15)$$

on the Fermi surface. Here s is the subdominant s -wave component. A simple way to include band anisotropy is to introduce anisotropic effective masses^{11,34} with $m_b < m_a$ in an infinite

band model. This gives an ellipsoidal Fermi surface which can always be mapped onto a circular one by scaling of momentum variables. At the same time the gap is transformed to^{11,34}

$$\Delta(\phi) = \Delta_0 \left(s + \frac{\alpha + \cos 2\phi}{1 + \alpha \cos 2\phi} \right). \quad (16)$$

There are no additional changes and the calculations proceed as before with Eqs. (11) and (12). For the direction $\beta = 0^\circ$, they are replaced by:

$$\omega = \Delta_0 \left[\frac{\nu}{\rho} \frac{1 + \alpha}{\sqrt{1 - \alpha}} \sin \phi \pm \left(\frac{\alpha + \cos 2\phi}{1 + \alpha \cos 2\phi} + s \right) \right], \quad (17)$$

and

$$\frac{d\omega}{d\phi} = 0 = \frac{\nu}{\rho} \frac{1 + \alpha}{\sqrt{1 - \alpha}} \cos \phi \mp \frac{2(1 - \alpha^2) \sin 2\phi}{(1 + \alpha \cos 2\phi)^2}, \quad (18)$$

with α the effective mass anisotropy parameter defined as^{11,34} $\alpha = (m_b - m_a)/(m_a + m_b)$. Again, for a general winding angle numerical solutions are needed although analytic ones are still possible in the limit $\nu/\rho \rightarrow 0$ in some cases. If we restrict ourselves to solutions of Eq. (16) which have at least some positive values for the critical frequency ω_c in the range $\nu \leq \rho \leq 1$ then we get for $\beta = 0^\circ$, and the critical angles $\phi_c = \pm\pi/2$ the following three solutions of Eq. (17)

$$\frac{\omega_c}{\Delta_0} = \begin{cases} \frac{\nu}{\rho} \frac{1 + \alpha}{\sqrt{1 - \alpha}} \pm (1 - s), & \phi_c = \frac{\pi}{2} \\ -\frac{\nu}{\rho} \frac{1 + \alpha}{\sqrt{1 - \alpha}} + (1 - s), & \phi_c = -\frac{\pi}{2} \end{cases} \quad (19)$$

without restrictions on the value of ν/ρ , and another solution

$$\frac{\omega_c}{\Delta_0} = 1 + s + \frac{1}{2} \left(\frac{\nu}{2\rho} \right)^2 \frac{(1 + \alpha)^3}{(1 - \alpha)^2}, \quad (20)$$

which is valid only for $\nu/\rho \rightarrow 0$ and corresponds in that case to ϕ_c near zero radians.

First we note the well known limit of $\nu = 0$ (no magnetic field) in which case the van Hove singularity in the density of states is split by the existence of the subdominant s -wave component of the gap and there are two singularities in the density of states positioned at $\omega_c = \Delta_0(1 \pm s)$. This holds whatever the value of the effective mass anisotropy α might be.

This mass anisotropy does not lead to a corresponding splitting of the van Hove singularities in the density of states. In a previous paper Schürer et al.³⁴ have considered the specific case of optimally doped YBCO and have suggested that reasonable model parameters are $\alpha = 0.4$ to account for a factor of a little more than 2 in the effective conductivity between b - and a -direction. Further consideration of finite temperature penetration depth data³⁵ suggests $s = -0.25$. This gives agreement between the model and the measured penetration depth data at low but finite temperatures T .

In the top frame of Fig. 5 we show results for $N_L(\rho, \omega)$ for a case with $\alpha = 0.4$, $s = -0.25$, and $\beta = 0^\circ$, i.e. in the antinodal direction. The top frame is a three dimensional plot of $N_L(\rho, \omega)$ vs. ρ and ω and is to be compared with the top frame of Fig. 1 (tetragonal case). We note striking differences in the ridge structure. Now, the two ridges at $\rho = 1$ and about $\omega = \Delta_0(1 \pm s)$ come together as the vortex core is approached and they eventually cross each other before diverging in the opposite direction. The contours for the critical frequencies, ω_c , are shown in the bottom frame of Fig. 5. The two ridges that cross are the solutions of Eq. (19) for $\phi_c = -\pi/2$ and of Eq. (20). The solution of Eq. (19) for $\phi_c = \pi/2$ and the plus sign gives the higher energy ridge shown in the top frame of Fig. 5 (and dash-dotted line in the bottom frame of this figure).

As in the tetragonal case (Fig. 4) the ridge topology in the LDOS changes considerably as the position of the STM tip is changed. We illustrate this in the top frame of Fig. 6 where we present results for a winding angle $\beta = 45^\circ$. Now all four ridges are seen in the entire range $\nu \leq \rho \leq 1$ and two cross overs can be observed. The contours of the critical frequencies ω_c , are shown in the bottom frame of Fig. 6. A comparison of the top frame of this figure with the top frame of Fig. 4 (tetragonal case, $\beta = 45^\circ$) makes the splitting of the van Hove singularity as a result of the subdominant s -wave component of the gap particularly transparent.

IV. LOCAL IMPURITY SCATTERING RATE

Finally, it is of interest to discuss briefly the local impurity scattering rates which are modified by the presence of supercurrents. Similar work has already appeared in a paper by Barash and Svidzinskii.²⁷ In Born approximation $\Im \tilde{\omega}(\rho, \beta, \omega)$ given by Eq. (4) is given by

$$\Im \tilde{\omega}(\rho, \beta, \omega) = \pi t^+ \Re \Omega(\rho, \beta, \omega), \quad (21)$$

where $\Re \Omega(\rho, \beta, \omega)$ is just the LDOS of Eq. (3) modified by the impurity scattering and plotted already in the top frame of Fig. 1 for the antinodal direction and in Fig. 3 for the nodal direction. It is clear then that the Doppler shift accounting for the supercurrents significantly affects the local scattering rates in the same way as they modify the LDOS. The changes due to the supercurrents are very different when unitary scattering is considered. In this case, we find from Eq. (5),

$$\Im \tilde{\omega}(\rho, \beta, \omega) = \pi \Gamma^+ \Re \left\{ \frac{\Omega(\rho, \beta, \omega)}{\Omega^2(\rho, \beta, \omega) + D^2(\rho, \beta, \omega)} \right\}. \quad (22)$$

For a fixed winding angle β defining $\gamma(\rho, \omega) = \Im \tilde{\omega}(\rho, \beta, \omega)$ we have for $\nu = 0.1$, $\mathbf{H} \parallel c$ -axis, and $\beta = 0^\circ$ the results shown in the top frame of Fig. 7 where we give a three dimensional plot of $\gamma(\rho, \omega)$ as a function of distance ρ from the vortex core and of energy ω for a system of tetragonal symmetry. This quantity is strikingly different from its Born limit counterpart which just corresponds to the $N_L(\rho, \omega)$ as plotted in the top frame of Fig. 1 scaled by a constant factor of πt^+ .

The $H = 0$ case in the unitary limit is quite similar to the $H \neq 0$ case at $\rho = 1$. The only difference is that for $H = 0$ there is only one shallow dip at $\omega = \Delta_0 = 24$ meV which does not change position as one moves from $\rho = 1$ to $\rho = \nu$. It is quite important to notice that in the limit $\omega \rightarrow 0$ $\gamma(\rho, \omega)$ decreases by almost one order of magnitude as one approaches the vortex core. This means that the supercurrents surrounding the vortex core will also influence substantially the value of the universal limit for the transport.

The equivalent results for a system with orthorhombic symmetry with an effective mass anisotropy parameter $\alpha = 0.4$ and an s -wave component $s = -0.25$ to the gap are shown in

the bottom frame of Fig. 7 to contrast the results for the system with tetragonal symmetry. The variation of $\gamma(\rho, \omega)$ in the limit $\omega \rightarrow 0$ is less dramatic in this particular case.

It is obvious from these results that the supercurrents modify significantly the local effective impurity scattering which depends strongly on ρ . This has already been emphasized by Barash and Svidzinskii²⁷ in another context.

V. CONCLUSION

In this work we have described the effect of supercurrents around the vortex core on the LDOS and on the local impurity scattering. We have included in the work only the effect of the Doppler shift in a semiclassical approximation on the extended quasiparticles. The work was motivated by the considerable success such an approach has had recently in describing the effect of vortex cores on the thermodynamics and some transport properties of *d*-wave superconductors for magnetic fields in the range $H_{c1} < H \ll H_{c2}$, between the lower and upper critical fields. The calculations predict definite modifications of the expected van Hove singularity at the gap amplitude Δ_0 in a *d*-wave superconductor. There are additional ridges which depend on the geometry of the STM arrangement, i.e. its distance from the vortex core and direction of the STM with respect to nodal or antinodal direction. They also depend on orthorhombicity and are modified by impurity scattering. So far we are not aware of experiments which confirm these predictions. We hope our work will stimulate more experiments. Of course more sophisticated approaches to the structure of a vortex core in a *d*-wave superconductor are possible.^{29–31} We have already mentioned the work of Franz and Tešanović.²⁶ They compare results for the LDOS obtained from a semiclassical approach with results from solutions for a single vortex within a BdG self consistent approach. For the angular averages over the vortex winding angle they consider, they do find good agreement between the two sets of results. An important additional aspect of these author's work is that they investigate the possibility that the tunneling matrix element may have angular dependence and that consequently STM does not directly measure the LDOS. In the particular model considered, the perpendicular tunneling is modulated

by a $\cos^2 2\phi$ in-plane dependence which strongly affects the low energy part of the STM spectrum because there can be no tunneling right on the diagonal of the Brillouin zone. This modulation, however, will have less effect away from the $\omega \sim 0$ region and is not important for the ridges. Here our own emphasis has been on the topology of the secondary van Hove ridges introduced in the LDOS by supercurrents. We have derived simple formulas for the position of these ridges in configuration space, for their dependence on H which varies with position about the vortex, and have examined the effect of impurities both in Born and in unitary scattering limit on the topology of the ridges. We have also considered the modifications that are introduced when orthorhombicity is introduced within an anisotropic effective mass model.

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FIGURES

FIG. 1. The top frame is the local density of states $N_L(\rho, \omega)$ as a function of energy ω and the distance from the vortex core ρ for a magnetic energy $E_H = \nu \Delta_0$ with $\nu = 0.1$ and a vortex winding angle $\beta = 0^\circ$ along the antinode in the d -wave gap. A small amount of elastic impurity scattering in Born approximation has been included with $t^+ = 0.1$ meV. The main ridge around 24 meV is the usual van Hove singularity at the gap amplitude Δ_0 modified only slightly by the magnetic field H . The other two ridges are due to the Doppler shift of the semiclassical approximation resultant from the existence of the supercurrents about the vortex core. The bottom frame is the density of states when $H = 0$ and is for comparison.

FIG. 2. The top frame gives the critical values of frequencies $\omega_{ci}, i = 1, 2, 3$ defining the three ridges in the top frame of Fig. 1. The bottom frame represents the same data as in the top frame of Fig. 1 but gives $N_L(\rho, \omega)$ vs. ω for several values of ρ , namely $\rho = 0.2$ (solid line), $\rho = 0.3$ (dashed line), $\rho = 0.6$ (dotted line) and $\rho = 1$ (dash-dotted line). Here, $\rho = 0.1$ corresponds to the vortex core radius equal to the coherence length ξ_0 and $\rho = 1.0$ the vortex cell of Radius R . Included is also, for comparison, $N(\omega)$ for $\nu = 0$, i.e. no magnetic field, as a thin solid line.

FIG. 3. The top frame shows a three dimensional plot of the LDOS $N_L(\rho, \omega)$ as a function of distance from the vortex core ρ in the vortex unit cell, and of frequency ω . Here the vortex winding angle is $\beta = 45^\circ$, i.e. the STM tip is moved along the nodal direction, and the magnetic energy is $\nu = 0.1$. The bottom frame gives the critical frequency $\omega_{ci}, i = 1, 2$ and the corresponding critical angles ϕ_{ci} that locate the ridges in the top frame as a function of the distance from the vortex core ρ , for $\nu = 0.1$, $\mathbf{H} \parallel c$ -axis, $\beta = 45^\circ$.

FIG. 4. A three dimensional plot of the LDOS as a function of the distance ρ from the vortex core in the vortex unit cell, and of frequency ω . Here the magnetic energy is $\nu = 0.1$, $\mathbf{H} \parallel c$ -axis, and the vortex winding angle $\beta = 0^\circ$ (antinode direction). Unitary impurity scattering is included with $\Gamma^+ = 0.1$ meV as compared to the top frame of Fig. 1 where the Born limit is used instead.

FIG. 5. Top frame: a three dimensional plot of the LDOS $N_L(\rho, \omega)$ as a function of distance from the vortex core ρ in the vortex unit cell, and of frequency ω . Here the vortex winding angle $\beta = 0$ (antinodeal direction) and $\mathbf{H} \parallel c$ -axis, i.e. perpendicular to the copper oxide planes. The mass anisotropy $\alpha = 0.4$ and an s -wave component $s = -0.25$ are included to model the orthorhombicity of YBCO. Born impurity scattering with $t^+ = 0.1$ meV is also included. The bottom frame gives the critical frequencies ω_c defining the van Hove ridges in the top frame.

FIG. 6. The top frame shows a three dimensional plot of the LDOS $N_L(\rho, \omega)$ as a function of distance from the vortex core ρ in the vortex unit cell, and of frequency ω . Here the vortex winding angle $\beta = 45^\circ$ and $\mathbf{H} \parallel c$ -axis. The effective mass anisotropy $\alpha = 0.4$ and an s -wave component $s = -0.25$ are included to model the orthorhombicity of YBCO. Born impurity scattering with $t^+ = 0.1$ meV is also included. The bottom frame gives the critical frequencies ω_c defining the van Hove singularities in the top frame.

FIG. 7. Top frame: the impurity scattering rate $\gamma(\rho, \omega)$ in the unitary limit with $\Gamma^+ = 0.1$ meV as a function of the distance from the vortex core ρ , and frequency ω . Here the magnetic energy $\nu = 0.1$, $\mathbf{H} \parallel c$ -axis, and the vortex winding angle $\beta = 0^\circ$, i.e. the STM tip is moved along the antinodeal direction. A system of tetragonal symmetry is considered. Bottom frame: the same as the top frame but for a system of orthorhombic symmetry having an effective mass anisotropy $\alpha = 0.4$ and an s -wave component $s = -0.25$ to model YBCO.













